

Heptafluorobutyric acid
375-22-4 | DTXSID4059916

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -14.1 °C

Global applicability domain: Inside

Local applicability domain index: 3.97e-01

Confidence level: 8.42e-01

Nearest Neighbors from the Training Set

Image not found

Heptafluorobutyric acid

Measured: -17.5

Predicted: -14.1

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1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: -4.00

Predicted: -8.02

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Acetic acid, trifluoro-

Measured: -15.2

Predicted: -15.5

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Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-

Measured: 34.0

Predicted: 32.9

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1-Propanol, 2,2,3,3-tetrafluoro-

Measured: -15.0

Predicted: -15.0